substance: boron compounds with group VI elements
property: properties of boron-oxygen compounds: $(BO)_x$, B_2O_3

On the interaction of oxygen (and hydrogen) with boron powder and the kinetics of removal of the gases [81T].

Ab initio studies of boron oxides (B_2O, B_2O_2, B_2O_3, B_3O_3, B_mO_n) with natural bond analysis [93N].

Quantitative electron probe microanalysis of ultralight elements boron-oxygen [90B].

$(BO)_x$

Preparation [77G], crystalline structure [77G]

Study of the boron-oxygen units in crystalline and molten barium metaborate by high temperature Raman spectroscopy [93V].

IR and Raman spectra of isotope-marked tetra- and pentaborates [80J].

FT-IR and Raman spectrocopic study of hydrated borates [95J] (FT-IR and Raman spectra of 27 hydrated borates are recorded and reexamined).

The nature of paramagnetic centers in gamma-irradiated boron oxide [90G].

B_2O_3

Preparation [77G], crystalline structure [77G, 71S2, 70G1, 68S], Raman and IR spectra [71B1, 71B2, 71S1, 60P], stimulated Brilloum scattering [71G], nuclear magnetic resonance [76R]

The crystal structure shows two polymorphs I and II with different coordination numbers of the boron atoms in Fig. 1 [68P, 70G1, 95T].

Calculated "Murnaghan" curve for types I and II in Fig. 2 [95T].

Ab initio total-energy pseudopotential calculation for polymorphic B_2O_3 crystals [95T].

Electronic structures and optical properties of low- and high-pressure phases of crystalline B_2O_3 [96D].

B_2O_3 crystals investigated by plane-wave pseudopotential calculations using the generalized-gradient approximation [97E].

Resonant X-ray Raman scattering in B K_α emission spectra of boron oxide (B_2O_3) excited by undulator radiation [93M].

Selectively excited B K_α emission spectra of B_2O_3 using undulator radiation [94K].

XANES spectrum in Fig. 3 [98M].

comparison between Raman and IR resonance wavenumbers for vitreous B_2O_3 [80W]

(ν/c in cm^{-1})

Raman	IR	IR	IR	
[80W]	[60P]	[63B]	[72T]	
21(3)				
120(20)				
~ 260				
400(10)				polarized
460(5)	464	463	465	
490(5)	500	503		
585(5)				polarized
650(5)		654	650	
725(5)	717…727	715	720	
801(3)	808			sym. breathing boroxol ring
	947			
1040(10)	1035			
	1094			
1200(10)				
1250(3)	1266	1258	1265	
1320(5)				
	1400	1407	1400	
1470(10)				
1460(25)				
1615(15)				deformation BOH
1996(25)				
2170(25)				
2640(15)				
2820(25)				
3540…3555				stretching OH
3595…3615				stretching OH

Vibrational spectra and the structure of pure vitreous B_2O_3 in Fig. 4 [80G].

IR absorbance at temperatures up to 1250 °C; room temperature data in Fig. 5 [87O].

Raman spectra of vitreous and molten B_2O_3 in [80W].

The molecular structure and computed vibrational spectrum of B_2O_3 in [81S].

Structural and vibrational model for vitreous boron oxide in [90B].

Ab initio calculations of structures, and Raman and infrared spectra of vitreous B_2O_3 [95Z].

density

(in g cm^{-3})

d	2.56	*T* = 300 K	type I	95T
	3.11		type II	
	1.84…1.91		glass	

Temperature dependence of the specific volume in Fig. 6 [66M, 65N, 99Z].

bulk modulus
(in GPa)

B_0	26	T = 300 K	Type I, calculated	95T
	47		type I empirical	
	126		type II, calculated	
	97		type II, empirical	
	15		glass, empirical	
	15		glass, experimental	

Temperature dependence of the infinite longitudinal frequency and shear moduli in Fig. 7 [66C, 99Z].

Temperature dependence of the longitudinal and transverse sound velocities Fig. 8 [89G, 99Z].

characteristic temperatures

T_g	532 K	glass transition temperature	99Z
T_m	723 K	melting point	99Z

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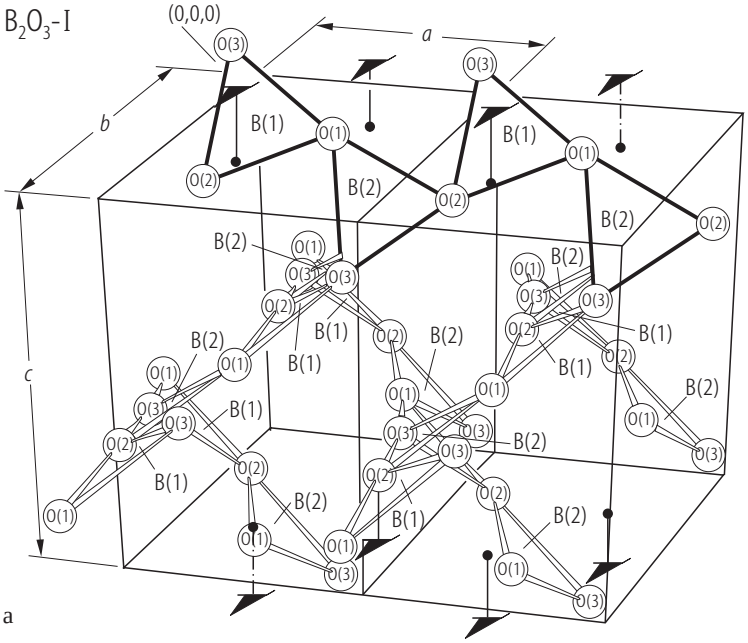
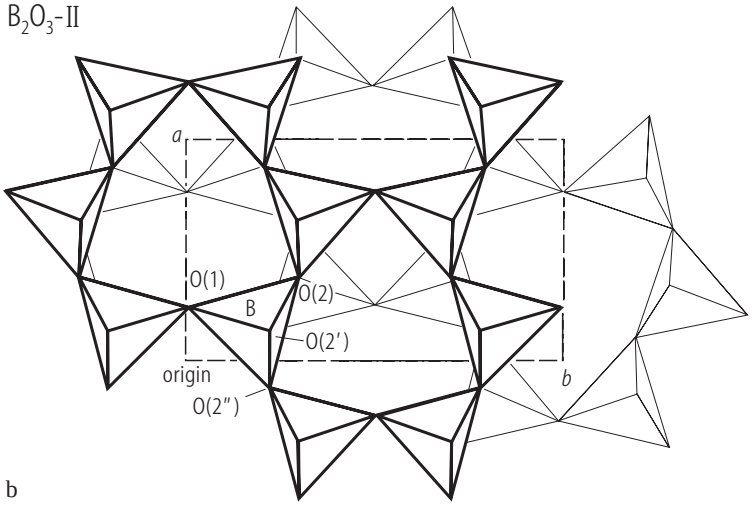
Fig. 1.

B_2O_3. Polymorphs of the crystal structure. **(a)** B_2O_3-I [70G2, 95T] and **(b)** B_2O_3-II [68P and 95T].



a



b

Fig. 2.

B_2O_3. Calculated "Murnaghan" curves for B_2O_3 –I and B_2O_3–II [95T].

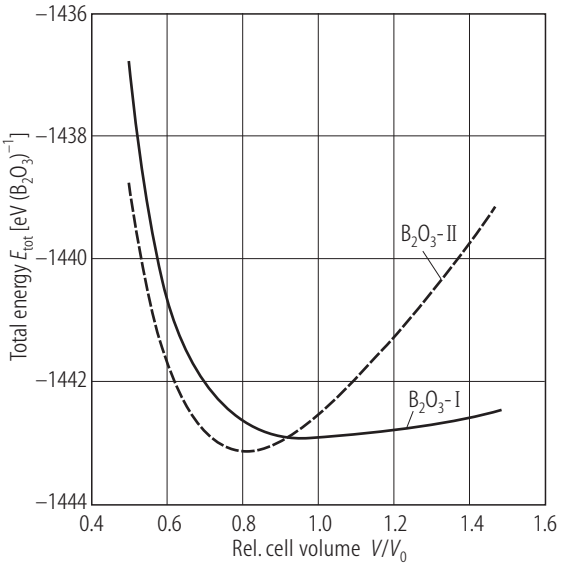


Fig. 3.

Al_3BC_3. XANES spectrum compared with those of some other boron compounds (boron carbide, B_2O_3, hexagonal BN) [98M].

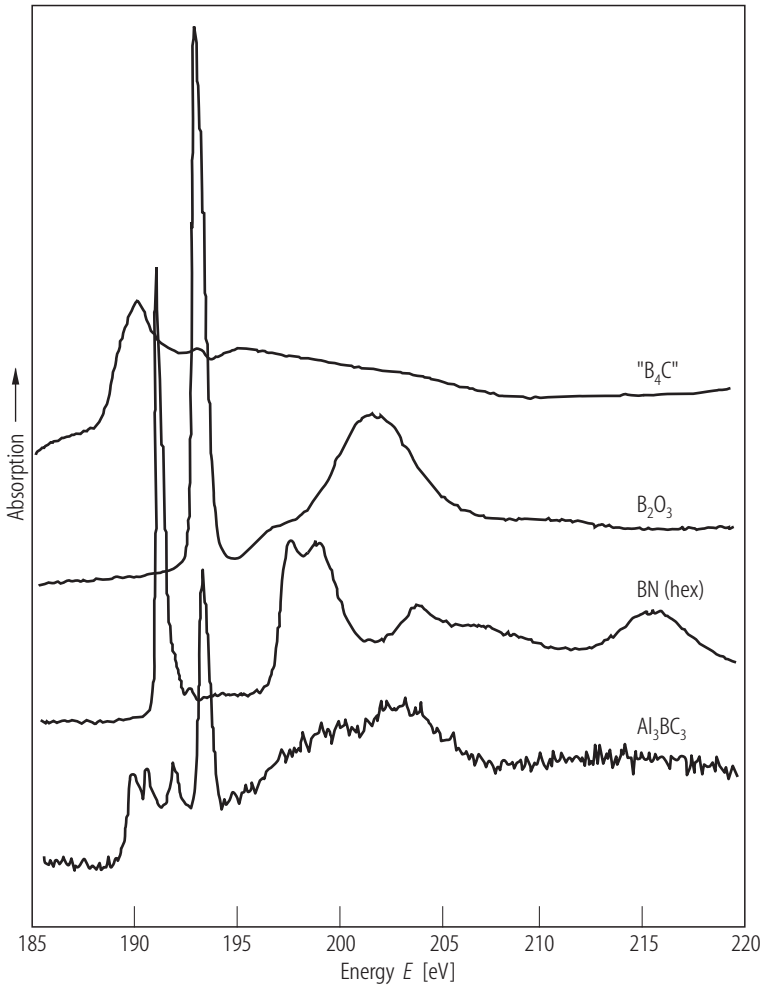


Fig. 4.

vitreous B_2O_3. (Top) Reduced Raman spectra, (middle) real and imaginary part of the dielectric function, (bottom) energy loss function. Vertical lines indicate the position of peaks in ε_2 and Im($-1/\varepsilon$) [80G].

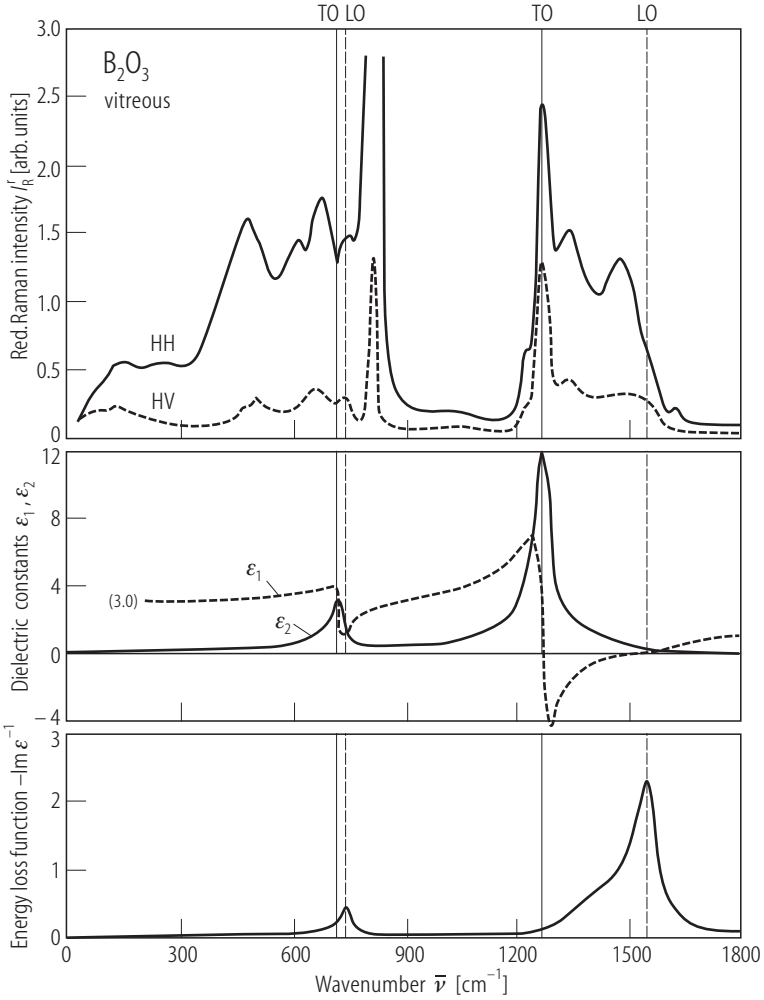


Fig. 5.

B_2O_3 films. Absorbance spectra at room temperature. Film thicknesses: *(1)* 1 μm, *(2)* 25 μm, *(3)* 75 μm [87O].

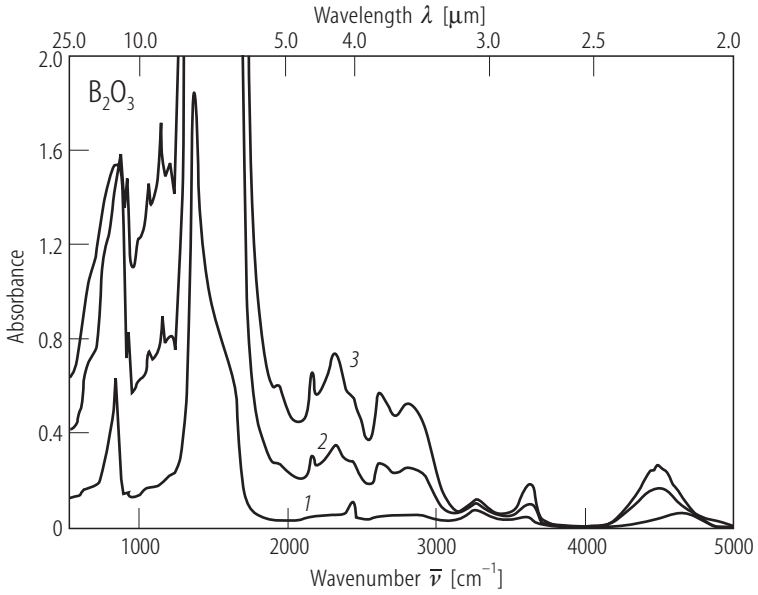


Fig. 6.

B_2O_3. Specific volume vs. temperature; circles, experimental results [66M, 65N], line, calculated [99Z]; T_g = glass transition temperature; T_m = melting temperature.

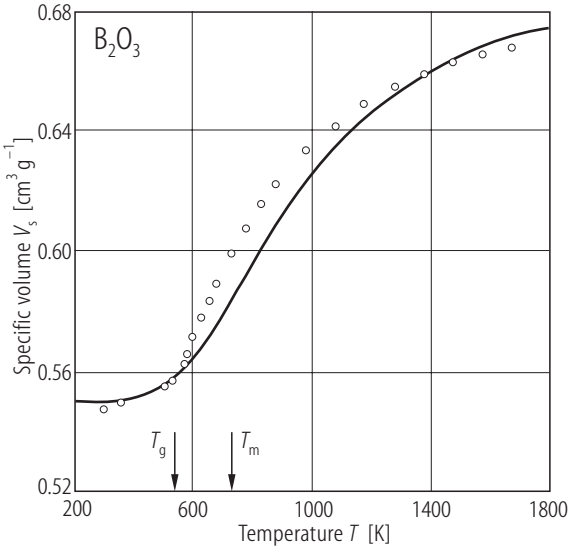


Fig. 7.

B_2O_3. Infinite longitudinal frequency and shear modulus vs. temperature. Circles, experimental results [66C], lines, calclated [99Z]. T_g = glass transition temperature; T_m = melting temperature.

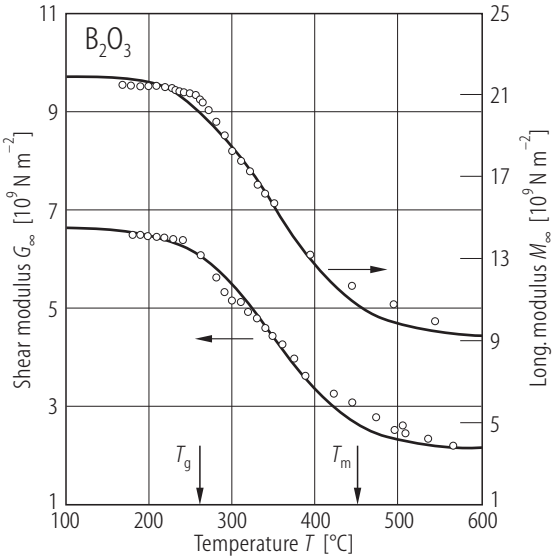


Fig. 8.

B_2O_3. Longitudinal and transverse sound velocities vs. temperature. Circles, experimental results [89G, 99Z]; lines, calculated [99Z]. T_g = glass transition temperature; T_m = melting temperature.